Supporting Information

Enhanced Reactivity in Dioxirane C-H Oxidations via Strain Release: A Computational and Experimental Study

Lufeng Zou,[1] Robert S. Paton*,[1,2] Albert Eschenmoser,[3] Timothy R. Newhouse,[4] Phil S. Baran,[4] and K. N. Houk*,[1]

[1] *Department of Chemistry and Biochemistry, University of California, Los Angeles, California 90095*

[2] *Chemistry Research Laboratory, Mansfield Road, Oxford, OX1 3TA U.K.*

[3] *Laboratorium für Organische Chemie, ETH Zürich, Wolfgang-Pauli-Strasse 10, CH-8093, Switzerland*

[4] *Department of Chemistry, The Scripps Research Institute, La Jolla, California 92037*

* houk@chem.ucla.edu, robert.paton@chem.ox.ac.uk

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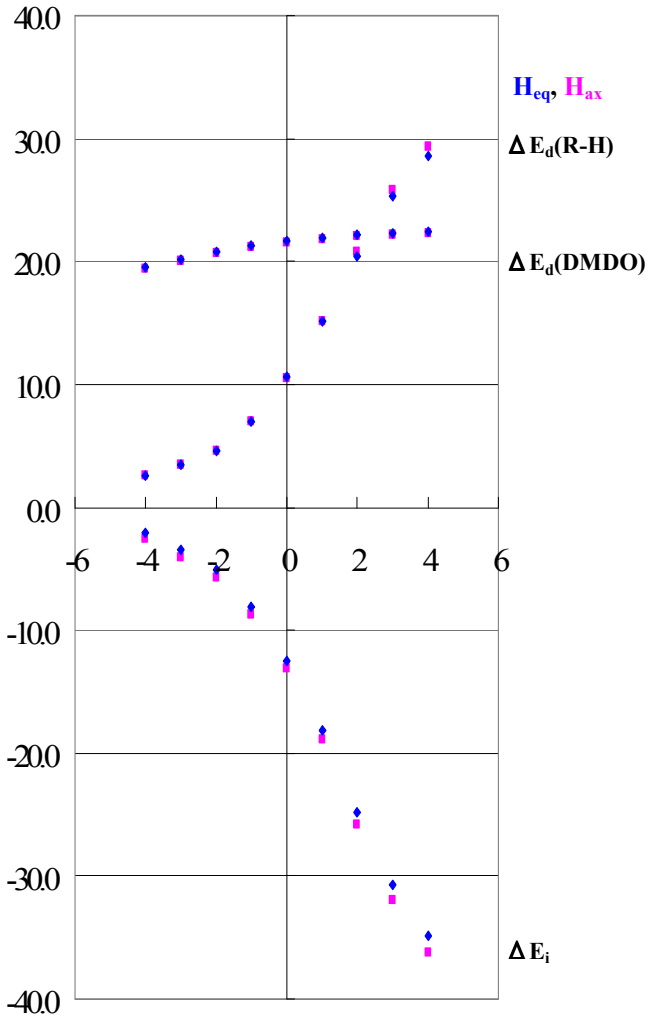

Figure S1. Breakdown of distortion/interaction energies along the internal reaction coordinates (IRC) for the reactions of DMDO with 1-methylcyclohexanes. The C-H bonds are functionalized at the equatorial position (for 1-axial-1-methyl-cyclohexane) or axial position (for 1-equatorial-1-methyl-cyclohexane). Energies in kcal/mol with respect to there corresponding reactants. The x axis is the "internal reaction coordinate" from calculation, and the origin is the transition state.

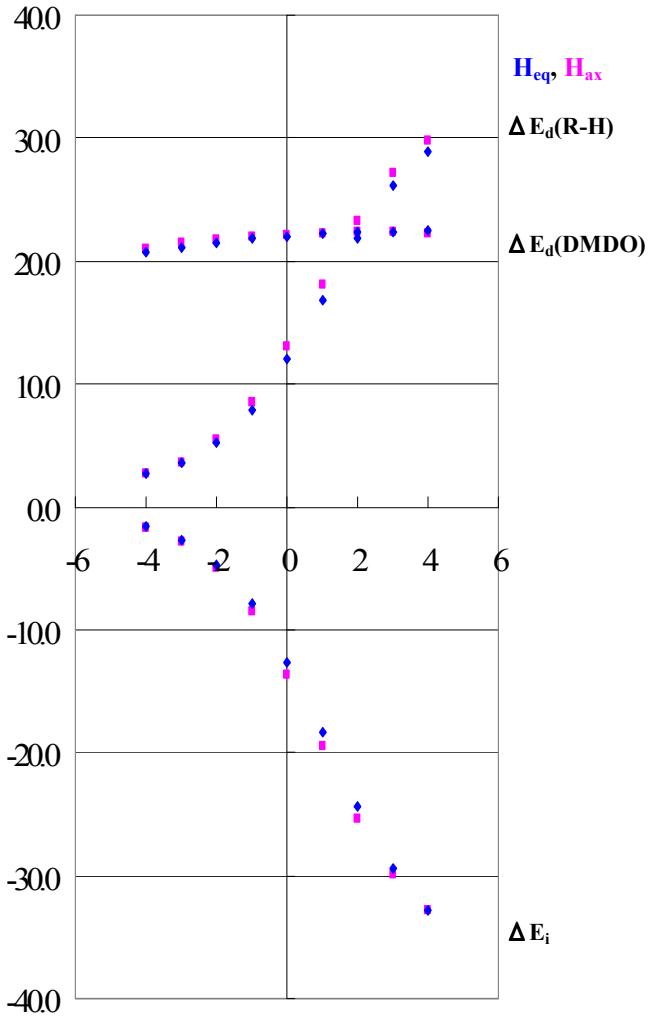

Figure S2. Breakdown of distortion/interaction energies along the internal reaction coordinates (IRC) for the reactions of DMDO with cyclohexanes. The C-H bonds are functionalized at the equatorial or axial positions. Energies in kcal/mol with respect to there corresponding reactants. The x axis is the "internal reaction coordinate" from calculation, and the origin is the transition state.

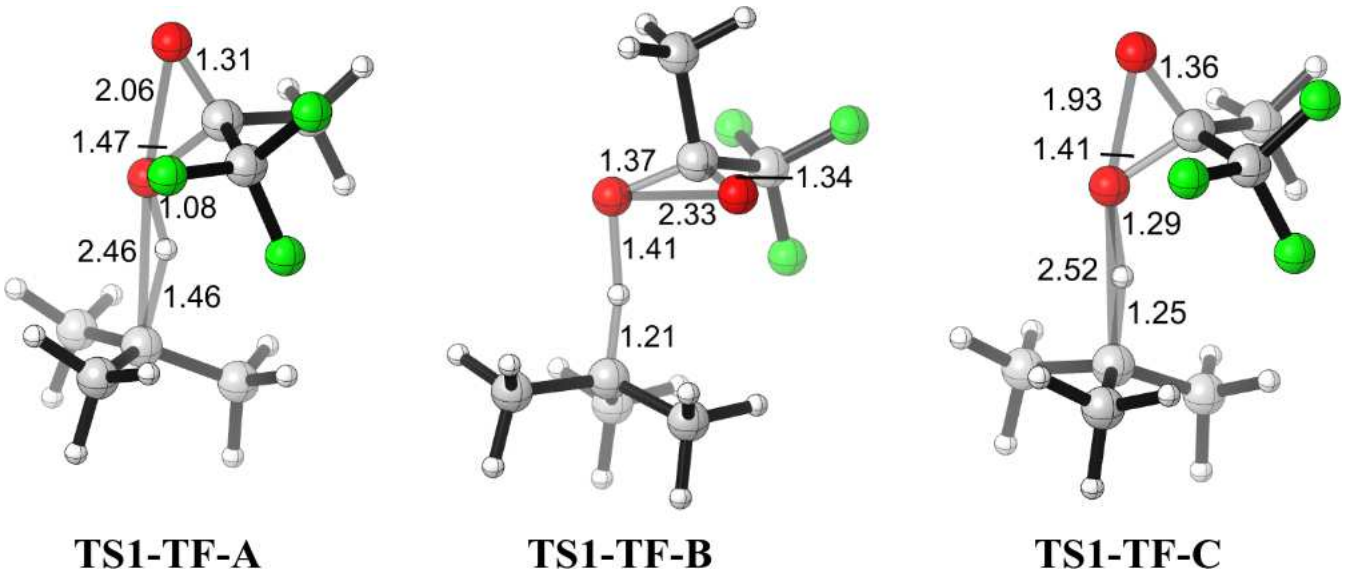

Figure S3. Transition state geometries for TFDO and isobutane reaction.

Table S1. Natural orbital occupancies (NOOs) of frontier orbitals, and activation energies in the rate-determining transition states[a]

	HOMO	LUMO	CASPT2/cc-pVDZ	CASPT2/6-31G(d)	UB3LYP[b]
TS1-A	1.42	0.58	21.0	28.3	19.9[c]
TS1-B	1.24	0.76	20.2	24.9	15.8
TS1-C	1.63	0.37	18.6	23.3	20.0
TS1-TF-A	1.53	0.48	11.6	16.3	8.9[d]
TS1-TF-B	1.20	0.80	17.9	21.4	11.1
TS1-TF-C	1.66	0.34	11.7	15.1	13.7

[a] cc-pVDZ basis set was exployed instead of cc-pVTZ in the text due to computational costs. The CASPT2 energies are less accurate but the NOOs are the same. CASPT2(10,10)/6-31G(d) or cc-pVDZ//UB3LYP/6-31G(d), energies in kcal/mol

[b] UB3LYP/6-311++G(d,p)//UB3LYP/6-31G(d)

[c] 24.2 kcal/mol with RB3LYP/6-311++G(d,p)

[d] 13.2 kcal/mol with RB3LYP/6-311++G(d,p)

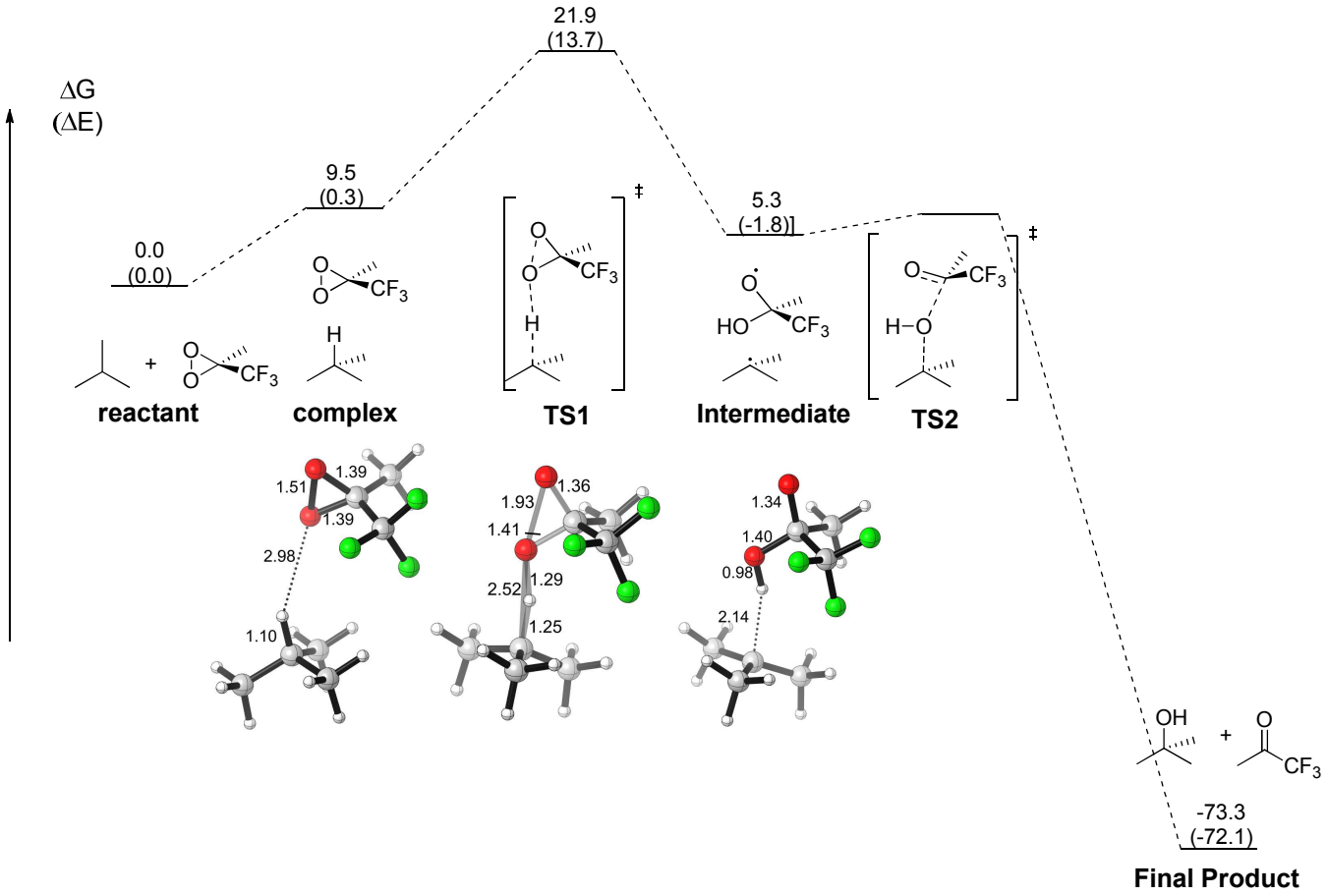

Figure S4. Reaction pathway in TFDO oxidations. Energy in kcal/mol. UB3LYP/6-311++G(d,p)//UB3LYP/6-31G(d).

The second TS has not been obtained. But it is expected to follow the same trend with low or no barrier as DMDO.

Cartesian Coordinates for Dioxiranes and Alkanes

DMDO:

O	-1.09041	-0.00558	0.75263
C	0.09370	0.00026	-0.00001
O	-1.09044	-0.00566	-0.75262
C	0.86539	1.29794	-0.00002
H	1.50689	1.36054	0.88623
H	1.50733	1.36030	-0.88597
H	0.16862	2.13859	-0.00030
C	0.87928	-1.28877	0.00002
H	1.52182	-1.34475	0.88617
H	0.19045	-2.13635	0.00024
H	1.52146	-1.34494	-0.88639

TFDO:

O	1.38476	-0.88012	-0.75447
C	0.74142	0.09506	-0.00015
O	1.38444	-0.88021	0.75445
C	1.29799	1.49111	-0.00003
H	0.95647	2.03235	-0.88747
H	0.95549	2.03262	0.88689
H	2.38799	1.43588	0.00059
C	-0.78696	-0.02042	-0.00005
F	-1.28642	0.59694	1.09211
F	-1.20085	-1.28622	-0.00117
F	-1.28699	0.59897	-1.09077

***t*Bu-TFDO:**

O	0.12709	1.68599	-0.76305
C	0.00643	0.52163	-0.00167
O	0.04750	1.69957	0.74088
C	-1.32297	-0.25258	-0.00539

C	1.34574	-0.24494	0.00791
F	1.34249	-1.25282	0.90799
F	2.36919	0.56056	0.29588
F	1.56417	-0.78333	-1.21021
C	-1.60757	-0.72982	1.43810
H	-2.57841	-1.23624	1.46539
H	-0.85132	-1.43070	1.79923
H	-1.65275	0.11911	2.12885
C	-2.44609	0.70532	-0.45089
H	-2.31742	1.02055	-1.49016
H	-3.40876	0.19030	-0.36471
H	-2.47721	1.60099	0.17542
C	-1.27065	-1.46036	-0.96468
H	-1.02888	-1.15345	-1.98766
H	-0.53935	-2.20973	-0.64977
H	-2.25470	-1.94062	-0.98234

Isobutane:

C	-0.39569	1.40733	0.09594
C	0.00012	0.00002	-0.37317
H	0.00007	0.00025	-1.47372
H	0.31302	2.16282	-0.26416
H	-1.39349	1.68304	-0.26613
H	-0.41256	1.46277	1.19251
C	-1.02120	-1.04624	0.09582
C	1.41685	-0.36109	0.09590
H	-0.76152	-2.04863	-0.26549
H	-1.06146	-1.08817	1.19243
H	-2.02974	-0.81022	-0.26466
H	1.47291	-0.37643	1.19247
H	1.71775	-1.35174	-0.26587
H	2.15452	0.36616	-0.26433

Cyclohexane (2):

C	-1.45730	-0.17163	-0.22934
C	-0.57991	-1.34752	0.22937
C	0.87722	-1.17588	-0.22942
C	1.45729	0.17162	0.22935
C	0.57991	1.34751	-0.22937
C	-0.87722	1.17589	0.22940
H	1.49412	-2.00271	0.14590
H	-0.60686	-1.41019	1.32770
H	-0.98717	-2.29519	-0.14628
H	-1.52515	-0.17943	-1.32764
H	-2.48173	-0.29227	0.14634
H	1.52512	0.17941	1.32766
H	2.48174	0.29227	-0.14630
H	0.98718	2.29518	0.14630
H	0.60689	1.41020	-1.32770
H	-0.91754	1.22998	1.32774
H	-1.49411	2.00270	-0.14595
H	0.91752	-1.22995	-1.32776

1,4-Dimethylcyclohexane (3):

C	-0.79029	1.26301	-0.64210
C	-1.62614	0.00001	-0.33997
C	-0.79029	-1.26300	-0.64217
C	0.57901	-1.26192	0.05766
C	1.39733	0.00002	-0.27145
C	0.57903	1.26198	0.05767
H	-2.48568	-0.00000	-1.02595
H	-0.62774	1.32450	-1.72826
H	-1.35627	2.16221	-0.36357
H	-0.62771	-1.32440	-1.72834
H	1.14334	-2.15835	-0.23340
H	1.58236	0.00006	-1.35844

H	1.14339	2.15839	-0.23341
C	-2.19756	-0.00005	1.08771
H	-2.82148	0.88585	1.25774
H	-2.82209	-0.88556	1.25745
H	-1.41415	-0.00041	1.85349
H	-1.35625	-2.16219	-0.36367
H	0.44654	-1.32681	1.14780
H	0.44660	1.32689	1.14782
C	2.75462	-0.00005	0.44050
H	3.34436	-0.88638	0.17635
H	3.34444	0.88624	0.17641
H	2.62608	-0.00008	1.53093

1,2-Dimethylcyclohexane (4):

C	0.38440	0.96260	-0.43367
C	0.86211	-0.51638	-0.46371
C	0.01715	-1.40560	0.46994
C	-1.48399	-1.31233	0.15623
C	-1.97479	0.14300	0.17563
C	-1.12623	1.02615	-0.75334
H	0.35439	-2.44754	0.38466
H	0.67866	-0.87104	-1.49099
H	0.91370	1.48681	-1.24382
H	-1.66951	-1.74035	-0.84039
H	-2.05914	-1.91986	0.86695
H	-3.02944	0.19221	-0.12469
H	-1.93053	0.53006	1.20331
H	-1.28029	0.69268	-1.79028
H	-1.47234	2.06754	-0.70830
H	0.19238	-1.11422	1.51582
C	2.36343	-0.67582	-0.19168
H	2.68291	-1.70952	-0.37123
H	2.95950	-0.02473	-0.84342

H	2.61723	-0.43126	0.84646
C	0.72519	1.70565	0.87051
H	1.80684	1.75855	1.03315
H	0.34967	2.73525	0.82964
H	0.28237	1.23182	1.75360

Axial methylcyclohexane (5):

C	-0.25252	1.26492	0.63125
C	0.95141	1.26952	-0.32561
C	1.80205	-0.00018	-0.16186
C	0.95117	-1.26956	-0.32572
C	-0.25254	-1.26471	0.63150
C	-1.13005	-0.00000	0.49385
H	0.60323	1.34240	-1.36553
H	1.56428	2.16218	-0.14545
H	0.12195	1.32149	1.66407
H	-0.86460	2.16333	0.47443
H	0.60257	-1.34224	-1.36553
H	2.25749	-0.00022	0.84012
H	1.56374	-2.16244	-0.14576
H	2.63139	-0.00017	-0.88099
H	0.12207	-1.32111	1.66424
H	-1.84413	0.00006	1.33021
H	-0.86463	-2.16330	0.47491
C	-1.96065	-0.00001	-0.80075
H	-2.60606	-0.88549	-0.85027
H	-2.60552	0.88586	-0.85034
H	-1.33502	-0.00025	-1.70012

diaxial 1,3-dimethylcyclohexane (6):

C	-0.00016	-0.73212	1.17657
C	-1.31759	-0.30919	0.48022
C	-1.26623	1.19006	0.11081

C	0.00037	1.56658	-0.67428
C	1.26666	1.18955	0.11099
C	1.31745	-0.30966	0.48036
H	-2.11382	-0.43417	1.22876
H	-0.00022	-0.27320	2.17612
H	-0.00037	-1.81854	1.34207
H	-1.28849	1.78306	1.03715
H	0.00068	2.64400	-0.88385
H	1.28918	1.78264	1.03727
H	2.11361	-0.43490	1.22893
H	2.16597	1.46599	-0.45570
C	1.71770	-1.19138	-0.71493
H	2.73751	-0.95108	-1.04018
H	1.69639	-2.25418	-0.44531
H	1.06188	-1.05880	-1.58051
C	-1.71816	-1.19094	-0.71483
H	-1.69813	-2.25363	-0.44461
H	-2.73757	-0.94978	-1.04059
H	-1.06182	-1.05965	-1.58015
H	-2.16538	1.46693	-0.45585
H	0.00029	1.06789	-1.65291

1,3,5-trimethylcyclohexane (7):

C	-1.42358	0.34963	-0.80782
C	-1.05133	-1.09615	-0.40130
C	0.40914	-1.40805	-0.80692
C	1.47520	-0.36238	-0.40095
C	1.01520	1.05797	-0.80707
C	-0.42373	1.45851	-0.40149
H	-1.68214	-1.75419	-1.01752
H	-1.49944	0.36802	-1.90489
H	-2.42601	0.59570	-0.43091
H	0.43127	-1.48367	-1.90398

H	2.36029	-0.58008	-1.01731
H	1.07000	1.11510	-1.90412
H	-0.67746	2.33413	-1.01761
H	1.72922	1.80279	-0.42917
C	-0.56419	1.94054	1.05340
H	0.11458	2.78098	1.24464
H	-1.58644	2.29099	1.24280
H	-0.34292	1.16921	1.79446
C	-1.40003	-1.45802	1.05348
H	-2.46775	-1.29110	1.24292
H	-1.19189	-2.51815	1.24430
H	-0.84445	-0.87939	1.79482
C	1.96345	-0.48217	1.05354
H	2.35511	-1.48920	1.24370
H	2.77602	0.23007	1.24364
H	1.18415	-0.29137	1.79462
H	0.69710	-2.39915	-0.42958

8:

C	-3.27801	0.62165	0.04864
C	-1.95213	-0.05724	-0.44042
C	-1.87641	-1.60130	-0.26541
C	-3.12375	-2.24389	-0.91187
C	-4.44266	-1.63939	-0.40912
C	-4.46828	-0.11710	-0.61306
H	-1.01017	-1.91674	-0.86107
H	-1.95122	0.09417	-1.53311
H	-3.06909	-2.10046	-2.00122
H	-3.11144	-3.32854	-0.74160
H	-5.28679	-2.09402	-0.94341
H	-4.44958	0.08945	-1.69371
H	-5.41096	0.30279	-0.23534
C	-1.62163	-2.13251	1.15847

H	-1.40480	-3.20670	1.10921
H	-0.76175	-1.64860	1.63305
H	-2.47988	-2.01015	1.82490
C	-3.47244	0.62322	1.58400
H	-2.60050	0.99815	2.12782
H	-4.32027	1.27019	1.84229
H	-3.69348	-0.37005	1.97880
H	-4.59123	-1.88520	0.65025
C	-0.71870	0.70147	0.07594
H	-0.62037	0.61907	1.15978
C	-3.25910	2.09129	-0.44632
H	-3.26593	2.09400	-1.54633
H	-4.18222	2.59484	-0.12860
C	-0.72775	2.17184	-0.35198
C	-2.03385	2.87658	0.04323
H	-2.04454	3.88937	-0.37800
H	-2.07509	2.99980	1.13293
H	0.13983	2.68300	0.08246
H	-0.60691	2.20557	-1.44366
O	0.46863	0.08877	-0.50878
C	1.47886	-0.24737	0.32568
O	1.48608	-0.11123	1.53593
N	2.49774	-0.81573	-0.40064
H	2.43237	-0.75806	-1.40762
C	3.77918	-1.08184	0.20038
H	4.18107	-2.04163	-0.14111
H	3.64369	-1.11903	1.28260
C	4.80907	-0.00986	-0.12472
F	4.44042	1.20172	0.32718
F	4.98723	0.09469	-1.46474
F	6.00157	-0.31918	0.42392

9:

C	-3.39959	0.69586	0.15058
C	-2.12132	-0.00446	-0.38199
C	-2.13903	-1.54073	-0.14426
C	-3.42082	-2.13632	-0.76545
C	-4.70016	-1.47415	-0.23398
C	-4.66129	0.04504	-0.44482
H	-1.28435	-1.95601	-0.69394
H	-2.10921	0.14455	-1.47481
H	-3.38199	-2.00238	-1.85671
H	-3.44892	-3.21916	-0.58634
H	-5.57900	-1.90031	-0.73464
H	-4.69007	0.25968	-1.52438
H	-5.55509	0.51480	-0.01266
C	-1.96900	-1.95880	1.32861
H	-2.02297	-3.05095	1.41395
H	-1.00046	-1.64793	1.73310
H	-2.74803	-1.54454	1.97830
H	-3.43192	0.56263	1.24370
H	-4.81998	-1.69445	0.83555
C	-3.36688	2.20897	-0.12857
H	-4.26060	2.68096	0.30073
H	-3.42054	2.37270	-1.21566
C	-0.86679	0.68922	0.16742
H	-0.77507	0.52998	1.24421
C	-2.09852	2.87397	0.42010
C	-0.84017	2.18870	-0.12987
H	-2.08361	3.94119	0.16760
H	-2.09753	2.81388	1.51802
H	-0.78077	2.33212	-1.21759
H	0.06639	2.62702	0.30440
O	0.29664	0.08051	-0.46477
C	1.32159	-0.29185	0.33587
O	1.35200	-0.20415	1.55016

N	2.32451	-0.83414	-0.43182
H	2.24126	-0.73317	-1.43411
C	3.61766	-1.12124	0.13355
H	3.50309	-1.20066	1.21589
H	4.01409	-2.06621	-0.25270
C	4.64003	-0.03551	-0.16916
F	4.27844	1.15735	0.33523
F	5.84276	-0.36329	0.34536
F	4.79328	0.12063	-1.50728

10:

C	-2.69943	-0.35986	-0.25468
C	-3.11687	1.06276	-0.71727
C	-2.34188	2.21122	-0.05920
C	-0.82503	2.04108	-0.22547
C	-0.30948	0.68116	0.31050
C	-1.14212	-0.46638	-0.38648
H	-2.96759	1.12431	-1.80571
H	-4.19468	1.19259	-0.54944
H	-0.57711	2.11866	-1.29468
H	-0.29548	2.86238	0.27606
H	-0.96914	-0.29253	-1.46168
H	-2.60381	2.28342	1.00401
C	-3.24459	-0.65470	1.15926
H	-4.34063	-0.69229	1.13245
H	-2.89730	-1.62581	1.53064
H	-2.96488	0.10134	1.89570
C	-0.36873	0.70419	1.85728
H	-0.43751	-0.28989	2.30310
H	0.52385	1.18901	2.26831
H	-1.22640	1.27447	2.22066
C	-3.37189	-1.36109	-1.22212
H	-3.26712	-2.39900	-0.88850

H	-4.44629	-1.15120	-1.29048
H	-2.95481	-1.28621	-2.23413
C	1.13097	0.45165	-0.20943
C	-0.55191	-1.87118	-0.10790
H	-1.13801	-2.62744	-0.63903
H	-0.63848	-2.12180	0.95680
C	1.76693	-0.92519	0.10309
C	0.92274	-2.01157	-0.55807
H	1.30165	-3.01134	-0.31335
H	0.99117	-1.89732	-1.64729
O	3.07619	-0.77617	-0.54181
C	3.47109	0.53403	-0.47922
O	4.56729	0.89231	-0.82226
C	2.08334	-1.27977	1.56481
H	2.80165	-2.10588	1.55751
H	2.54205	-0.44762	2.10709
H	1.20190	-1.60318	2.12122
C	2.30986	1.39454	0.03979
H	2.47709	1.63401	1.09724
H	2.27818	2.33677	-0.51196
H	1.02841	0.43574	-1.30523
H	-2.65259	3.16417	-0.50605

Cartesian Coordinates for Transition states

TS1-A:

C	1.79987500	-0.00033600	0.03360400
H	0.37475500	-0.39848300	-0.27379000
C	1.88103200	1.49676100	0.08875400
H	1.65141000	1.94678700	-0.87919100
H	1.20426100	1.91223800	0.84045400
H	2.90788100	1.78668900	0.36946000
C	1.87192800	-0.72621700	1.35198300

H	2.89939600	-0.64050300	1.74501000
H	1.20489800	-0.28441000	2.09929500
H	1.64884600	-1.79338900	1.25477100
C	2.42718800	-0.67021600	-1.15749800
H	2.21345600	-1.74291100	-1.18840600
H	2.08998800	-0.21260600	-2.09131800
H	3.52250200	-0.55109300	-1.10147600
O	-0.41343300	0.04210900	-0.80911600
C	-1.76654300	-0.00869800	-0.10886700
O	-2.44543000	0.12837300	-1.22281200
C	-1.85138200	1.17493200	0.86506200
C	-1.91121600	-1.37552500	0.58257100
H	-1.66712400	2.10055700	0.31357600
H	-2.85778900	1.22346500	1.29713000
H	-1.13369300	1.09138000	1.69268000
H	-2.92510200	-1.46898400	0.98743100
H	-1.76239600	-2.16673400	-0.15753900
H	-1.20566900	-1.51006600	1.41367500

TS1-B:

C	-1.74558700	-0.02612500	0.02628900
H	-0.57627500	-0.17818600	0.40860600
C	-2.54816800	-0.09304800	1.31771100
H	-2.36056600	-1.02881300	1.85502900
H	-2.30674200	0.74108800	1.98584400
H	-3.62564200	-0.04347200	1.09836200
C	-1.82839400	1.31666500	-0.68521200
H	-2.85157600	1.48096000	-1.05659000
H	-1.58987800	2.14862400	-0.01251000
H	-1.15262700	1.35555600	-1.54564100
C	-1.94378900	-1.22111000	-0.89465300
H	-1.23086700	-1.19512600	-1.72411200
H	-1.80569700	-2.16349200	-0.35426300

H	-2.96213400	-1.21645700	-1.31199400
O	0.62425400	-0.60565700	0.81628300
C	1.58994700	-0.03177200	-0.00564800
O	1.36316200	-0.11339900	-1.33552200
C	2.89093300	-0.84647800	0.31505100
C	1.81982600	1.47869900	0.32705800
H	2.73170400	-1.89252300	0.04628000
H	3.72117000	-0.43565000	-0.26395000
H	3.10216500	-0.77423000	1.38437700
H	2.66292700	1.87801300	-0.24143200
H	0.92196000	2.05158500	0.08253800
H	2.01414700	1.56357800	1.39979600

TS1-C:

C	-1.75165400	-0.00633900	0.01548700
H	-0.50608600	-0.02829600	-0.32757700
C	-2.09500100	1.46869100	-0.07171300
H	-1.52714800	2.06090500	0.65348500
H	-1.89674600	1.86348200	-1.07284900
H	-3.16453400	1.61553500	0.14315600
C	-2.37943000	-0.87070800	-1.06158100
H	-3.46949400	-0.91713400	-0.91541600
H	-2.19151500	-0.46191300	-2.05915800
H	-1.99352000	-1.89452600	-1.02986600
C	-1.79710800	-0.59569300	1.41212700
H	-1.41950500	-1.62324900	1.43110000
H	-1.22370900	0.00304300	2.12826800
H	-2.83879400	-0.62078400	1.76783000
O	0.56582500	-0.01738600	-0.91523000
C	1.71893900	0.00147700	-0.07078900
O	2.51273100	0.05932600	-1.18983000
C	1.89296500	-1.29663000	0.71875400
C	1.79504400	1.26418800	0.78913000

H	1.78950600	-2.14466700	0.03698900
H	2.89062900	-1.32940000	1.17141200
H	1.15490100	-1.38502200	1.52474700
H	2.78168900	1.34035800	1.26006900
H	1.64118100	2.13946500	0.15283100
H	1.04216500	1.25676600	1.58697400

TS1-TF-A:

C	-2.30715800	-0.12761600	0.03600900
H	-0.99026100	0.46776900	-0.13495000
C	-2.33011900	-0.18538300	1.53877500
H	-1.51864100	-0.80228200	1.93246000
H	-2.28714100	0.81032600	1.99049800
H	-3.28181500	-0.64746400	1.85179600
C	-3.14924200	0.92311200	-0.62842900
H	-4.20520200	0.60819800	-0.58138300
H	-3.06932200	1.89050700	-0.12497400
H	-2.88270900	1.04364200	-1.68144800
C	-2.11933400	-1.42306400	-0.69971200
H	-1.89129800	-1.25394700	-1.75489800
H	-1.32828900	-2.03025000	-0.25470500
H	-3.06049800	-1.99518200	-0.64272800
O	-0.21230400	0.89465600	-0.74422200
C	1.13393200	0.88571400	-0.15481700
O	1.71741300	1.47667300	-1.17121700
C	1.54886400	-0.60023900	0.01355200
C	1.17789700	1.63238700	1.18284000
F	2.81391800	-0.70296100	0.46524400
F	1.45101900	-1.29714600	-1.12514300
F	0.75138700	-1.24125300	0.93659500
H	2.21154900	1.68420800	1.53802900
H	0.81441500	2.64775700	1.00848500
H	0.57239000	1.14885700	1.95776400

TS1-TF-B:

C	2.25030100	-0.09408500	0.02097000
H	1.14095600	0.40204800	-0.25056600
C	2.18956700	-1.46117300	-0.63851500
H	1.39412100	-2.07714200	-0.21076100
H	2.02250700	-1.37520300	-1.71651700
H	3.14509200	-1.98484600	-0.48529800
C	3.21134000	0.88222700	-0.63510800
H	4.24479300	0.53129400	-0.49590400
H	3.02644400	0.96209200	-1.71072900
H	3.13477300	1.88116100	-0.19411100
C	2.31219100	-0.12220800	1.53852300
H	2.24699300	0.88397300	1.96616500
H	1.51519100	-0.74036700	1.96140200
H	3.27378400	-0.55364000	1.85491700
O	0.11499900	0.94967400	-0.81650400
C	-1.10674400	0.85965700	-0.11486000
O	-1.70360200	1.49017800	-1.15929900
C	-1.15639200	1.60119900	1.21366600
C	-1.55731200	-0.61353900	0.01407400
H	-0.80634800	2.62171300	1.04390300
H	-2.18578000	1.63254200	1.58375200
H	-0.53232700	1.11728200	1.97103900
F	-2.83444200	-0.68260900	0.44131900
F	-0.79054000	-1.27401400	0.93168900
F	-1.46047100	-1.28028700	-1.14005000

1-TF-C:

C	-2.28570100	-0.03879600	-0.02368300
H	-1.18521400	0.35114600	-0.33767000
C	-2.49340700	-1.31289000	-0.83184800
H	-2.42705300	-1.11949400	-1.90787100
H	-1.75401300	-2.07597800	-0.57109800

H	-3.49205000	-1.72696800	-0.62712100
C	-2.25914300	-0.25661100	1.48417200
H	-3.25638200	-0.56673700	1.83067500
H	-1.54814400	-1.03908000	1.76435700
H	-1.98710500	0.66111300	2.01461000
C	-3.17727800	1.11812400	-0.45670200
H	-2.91994100	2.03925500	0.07629300
H	-3.09387300	1.30755100	-1.53207400
H	-4.22943300	0.88376800	-0.23659100
O	-0.03245200	0.98772900	-0.84279500
C	0.99951400	0.80469000	0.04597100
O	0.79230600	1.14571900	1.32955100
C	2.14128600	1.77155800	-0.46170600
C	1.54001100	-0.66439900	-0.01862200
H	1.77390500	2.79449200	-0.38294300
H	3.02888100	1.62959500	0.15560000
H	2.34500800	1.51971400	-1.50370300
F	1.86812500	-1.00040500	-1.27805200
F	2.62841400	-0.82389200	0.75237700
F	0.60067200	-1.53748300	0.40767400

Reaction pathways of DMDO-isobutane:

Complex:

C	-2.27100	0.00599	-0.00315
H	-1.17939	-0.05481	-0.12585
C	-2.89526	0.04685	-1.40494
H	-2.55038	0.92058	-1.97107
H	-2.63639	-0.84886	-1.98165
H	-3.99054	0.10042	-1.34415
C	-2.72287	-1.24251	0.76700
H	-3.81110	-1.23954	0.91514
H	-2.46209	-2.15935	0.22553
H	-2.25329	-1.29326	1.75691

C	-2.59036	1.28614	0.78203
H	-2.12267	1.27445	1.77442
H	-2.23598	2.17955	0.25313
H	-3.67313	1.39629	0.92828
O	1.32429	-0.75653	-0.63826
C	2.25968	0.04914	0.02881
O	2.80959	-0.91843	-0.82671
C	2.41815	-0.21484	1.50652
C	2.35605	1.47779	-0.44969
H	2.32301	-1.28538	1.69922
H	3.39931	0.12904	1.85260
H	1.65231	0.32457	2.07511
H	3.33411	1.90013	-0.19342
H	2.22201	1.51018	-1.53282
H	1.58686	2.09425	0.02894

Intermediate:

C	-2.19424	0.00337	0.01177
H	0.00889	-0.10989	-0.38159
C	-2.21069	1.38339	-0.57957
H	-1.88025	2.14169	0.14034
H	-1.57052	1.45057	-1.46725
H	-3.22957	1.67127	-0.89856
C	-2.37807	-1.16096	-0.91838
H	-3.42992	-1.24640	-1.24907
H	-1.76927	-1.05789	-1.82425
H	-2.12109	-2.11299	-0.43872
C	-2.58020	-0.16538	1.45135
H	-2.26605	-1.13856	1.84860
H	-2.15491	0.62217	2.08580
H	-3.67719	-0.11415	1.58446
O	0.81273	-0.09910	-0.93602
C	1.95532	-0.01659	-0.09264

O	3.08006	-0.00311	-0.82432
C	2.01864	-1.25959	0.84518
C	1.91779	1.30377	0.73462
H	2.06657	-2.16450	0.23475
H	2.89575	-1.20889	1.49448
H	1.11283	-1.29281	1.46040
H	2.79592	1.37919	1.38011
H	1.89313	2.15374	0.04857
H	1.01203	1.31701	1.35061

Second TS:

C	2.06243	-0.00818	0.04490
H	-0.36114	0.61631	-1.27906
C	2.46398	1.22295	-0.69697
H	2.32281	1.11776	-1.77830
H	1.89998	2.09616	-0.34960
H	3.53363	1.44976	-0.53456
C	1.94587	0.06682	1.52903
H	2.94478	0.07401	2.00197
H	1.43671	0.98547	1.83977
H	1.40185	-0.79061	1.93777
C	2.17514	-1.34034	-0.61498
H	1.51124	-2.07657	-0.15073
H	1.94758	-1.28778	-1.68498
H	3.20426	-1.73605	-0.52756
O	-0.38553	0.40042	-0.33056
C	-1.80756	-0.01085	-0.14843
O	-2.44495	0.01165	-1.30795
C	-2.41722	1.06353	0.79817
C	-1.78465	-1.40357	0.51679
H	-2.41190	2.03082	0.29031
H	-3.44552	0.79623	1.05717
H	-1.81157	1.12762	1.70825

H	-2.81032	-1.71984	0.72976
H	-1.33530	-2.12422	-0.17299
H	-1.21122	-1.39781	1.44977

Acetone:

C	-0.00000	0.18532	-0.00000
O	0.00000	1.40098	0.00000
C	-1.29310	-0.61480	0.00001
H	-1.34131	-1.26754	0.88083
H	-2.14854	0.06354	0.00026
H	-1.34153	-1.26711	-0.88113
C	1.29310	-0.61480	-0.00001
H	1.34155	-1.26708	0.88115
H	1.34130	-1.26757	-0.88081
H	2.14853	0.06355	-0.00029

tBuOH:

C	0.68723	1.26751	-0.50955
C	-0.00545	-0.00002	0.01384
H	0.20346	2.16017	-0.09957
H	1.74411	1.28478	-0.21137
H	0.65163	1.32314	-1.60387
C	0.69417	-1.26347	-0.51017
C	-1.49037	-0.00394	-0.35739
H	0.21555	-2.15899	-0.10039
H	0.65862	-1.31890	-1.60449
H	1.75123	-1.27490	-0.21230
H	-1.62225	-0.00364	-1.44468
H	-1.98124	-0.89201	0.05409
H	-1.98612	0.88091	0.05517
O	0.01342	-0.00030	1.45234
H	0.94415	0.00136	1.72840

Reaction pathways of TFDO-isobutane:

Complex:

C	-2.69147	-0.14100	-0.07921
H	-1.88495	-0.38130	-0.78617
C	-2.79682	1.38831	0.00755
H	-1.85103	1.83156	0.33864
H	-3.04976	1.82614	-0.96573
H	-3.57698	1.68797	0.72011
C	-3.99123	-0.75830	-0.61320
H	-4.83210	-0.54479	0.06029
H	-4.24699	-0.35694	-1.60123
H	-3.90757	-1.84794	-0.70528
C	-2.31073	-0.74491	1.28050
H	-2.19573	-1.83371	1.21524
H	-1.36629	-0.32667	1.64738
H	-3.08207	-0.53551	2.03380
O	0.81321	-1.57933	-0.39298
C	1.80897	-0.67739	-0.03482
O	1.98106	-1.25038	-1.29039
C	2.75971	-1.05203	1.06712
C	1.37189	0.79142	-0.07637
H	2.99187	-2.11528	0.98514
H	3.68026	-0.46629	0.98513
H	2.30644	-0.84783	2.04177
F	2.45506	1.58267	-0.21763
F	0.77060	1.11971	1.09067
F	0.52531	1.04335	-1.07431

Intermediate:

C	2.61902	-0.08552	0.02311
H	0.64856	0.61079	-0.44176
C	2.47994	-1.28838	-0.86413
H	1.71980	-1.98338	-0.49087

H	2.21543	-1.00813	-1.89021
H	3.42942	-1.85196	-0.92129
C	3.30363	1.13007	-0.52981
H	4.39884	0.98435	-0.57566
H	2.97328	1.35441	-1.55075
H	3.13109	2.01676	0.09169
C	2.62575	-0.29755	1.50841
H	2.49112	0.64274	2.05741
H	1.84582	-1.00086	1.82230
H	3.58839	-0.72252	1.84815
O	-0.10962	0.96713	-0.95398
C	-1.29507	0.84765	-0.21163
O	-2.33345	1.40379	-0.84869
C	-1.20060	1.59134	1.16132
C	-1.59396	-0.66684	0.03644
H	-0.98444	2.64138	0.95890
H	-2.13266	1.49688	1.71897
H	-0.38006	1.14884	1.73397
F	-2.68532	-0.83952	0.79857
F	-0.54701	-1.24578	0.68533
F	-1.77126	-1.32373	-1.11522

Trifluoroacetone:

C	-0.90093	0.30755	-0.00000
O	-1.24455	1.46509	0.00001
C	0.61181	-0.03808	-0.00001
C	-1.82891	-0.88078	0.00001
H	-1.63958	-1.50424	-0.88137
H	-1.63924	-1.50453	0.88110
H	-2.86409	-0.53635	0.00025
F	1.37430	1.05367	-0.00030
F	0.91321	-0.77752	-1.09114
F	0.91331	-0.77701	1.09144

2-eq-TS:

O	-3.43913	-0.08999	-1.13131
C	-2.61080	-0.00187	-0.03337
O	-1.45313	-0.08228	-0.86420
C	2.93337	-1.26070	0.22380
C	1.44286	-1.28192	-0.20001
C	0.76206	-0.02158	0.28543
C	1.40492	1.26402	-0.18474
C	2.89560	1.28048	0.23945
C	3.62997	0.02345	-0.25050
H	-0.43723	-0.04206	-0.24900
H	1.38301	-1.32973	-1.29541
H	0.94418	-2.17508	0.19174
H	2.99873	-1.33014	1.31881
H	3.43759	-2.14757	-0.17954
H	1.34368	1.32336	-1.27950
H	0.88162	2.13806	0.21821
H	3.37378	2.18679	-0.15230
H	2.95873	1.33802	1.33527
H	3.66862	0.03072	-1.34933
H	0.52023	-0.03197	1.35516
C	-2.72050	1.34695	0.68213
H	-3.70814	1.44954	1.14603
H	-1.96603	1.44901	1.47183
H	-2.59059	2.14943	-0.04853
C	-2.73880	-1.20661	0.90236
H	-1.98179	-1.18418	1.69570
H	-3.72553	-1.21218	1.37922
H	-2.62496	-2.12414	0.31932
H	4.67009	0.03697	0.09902

2-ax-TS:

C	-0.83062	-0.11719	1.13506
C	-1.51411	1.21825	0.92441
C	-2.15747	1.32293	-0.46881
C	-3.05707	0.11337	-0.76764
C	-2.28860	-1.20983	-0.62404
C	-1.64285	-1.34191	0.76592
H	-2.29447	1.31604	1.69999
H	-0.80918	2.04077	1.09442
H	0.15056	-0.12019	0.27252
H	-0.27701	-0.20448	2.07634
H	-3.91546	0.11567	-0.07847
H	-2.43200	-1.45761	1.53007
O	0.93820	-0.12757	-0.63737
C	2.29467	0.00237	-0.20260
O	2.73074	-0.07466	-1.50511
H	-1.35680	1.37615	-1.21752
H	-2.73003	2.25535	-0.54281
H	-1.49685	-1.25651	-1.38258
H	-1.02251	-2.24380	0.82626
H	-2.95501	-2.06210	-0.80376
C	2.57026	1.36377	0.43897
H	2.09156	1.45281	1.42178
H	3.64834	1.50503	0.57641
H	2.19480	2.15089	-0.21998
C	2.74695	-1.18550	0.64905
H	3.83372	-1.15774	0.78720
H	2.28139	-1.17333	1.64197
H	2.48170	-2.11341	0.13594
H	-3.47131	0.19674	-1.77989

3-eq-TS:

O	-3.65785	0.04933	-1.50062
C	-3.06747	0.08350	-0.26188

O	-1.80025	-0.12675	-0.88706
C	2.55868	-1.22423	-0.24271
C	1.02532	-1.26523	-0.43695
C	0.34118	-0.18502	0.39115
C	0.89508	1.20427	0.10146
C	2.42888	1.23894	0.29529
C	3.14318	0.16661	-0.54601
H	-0.83455	-0.14936	-0.12696
H	0.79642	-1.09845	-1.49719
H	0.63274	-2.25516	-0.17748
H	2.81017	-1.50519	0.79068
H	3.02288	-1.97934	-0.89012
H	0.66134	1.47000	-0.93741
H	0.41372	1.95409	0.74053
H	2.80129	2.23734	0.03172
H	2.67237	1.08766	1.35718
H	2.94059	0.38769	-1.60619
C	-3.16685	1.45010	0.41791
H	-4.20630	1.65688	0.69728
H	-2.55887	1.49475	1.32998
H	-2.83096	2.22136	-0.27993
C	-3.48170	-1.08486	0.63377
H	-2.89192	-1.11684	1.55754
H	-4.53771	-0.98965	0.91144
H	-3.34601	-2.01971	0.08396
C	0.11846	-0.51786	1.85540
H	-0.48039	0.24999	2.35786
H	-0.38022	-1.48546	1.97575
H	1.07980	-0.57740	2.38662
C	4.66168	0.20142	-0.33526
H	5.16711	-0.54245	-0.96229
H	5.07483	1.18593	-0.58443
H	4.91991	-0.01326	0.70980

3-ax-TS:

C	-0.50501	1.06355	0.06205
C	-1.30909	0.84481	-1.21253
C	-1.86047	-0.58553	-1.34251
C	-2.62863	-1.05150	-0.08736
C	-1.72956	-0.89071	1.15715
C	-1.18200	0.53743	1.32031
H	-2.13804	1.57336	-1.20485
H	-0.69567	1.09620	-2.08652
H	0.48648	0.24912	-0.09422
H	-2.00239	1.23377	1.56507
O	1.24665	-0.69937	-0.30514
C	2.63365	-0.45711	-0.03960
O	2.89937	-1.75175	-0.40331
H	-1.01639	-1.26309	-1.51546
H	-2.50756	-0.64717	-2.22689
H	-0.87719	-1.57457	1.07003
H	-0.48633	0.58464	2.16757
H	-2.28082	-1.17612	2.06231
C	3.24326	0.57169	-0.99236
H	2.90970	1.58997	-0.76099
H	4.33634	0.55015	-0.91544
H	2.95905	0.31978	-2.01724
C	2.90679	-0.17416	1.43807
H	3.98508	-0.20107	1.63240
H	2.53631	0.81374	1.73743
H	2.42214	-0.94320	2.04499
H	-2.83070	-2.12491	-0.20765
C	0.12682	2.43488	0.19417
H	0.79218	2.49720	1.06240
H	0.69204	2.71044	-0.70253
H	-0.66064	3.19140	0.33165

C	-3.98834	-0.35142	0.06903
H	-4.61911	-0.52221	-0.81158
H	-4.52694	-0.73347	0.94451
H	-3.89013	0.73341	0.19420

4-eq-TS:

O	-3.37647	0.30465	-1.35326
C	-2.74533	-0.12933	-0.21538
O	-1.50434	0.31063	-0.77312
C	2.58745	-1.71584	0.12377
C	1.06760	-1.47854	-0.03721
C	0.69030	-0.05864	0.36974
C	1.46027	0.99758	-0.43278
C	2.98482	0.75954	-0.26816
C	3.39214	-0.66839	-0.65680
H	-0.49791	0.07837	-0.09253
H	0.79539	-1.63169	-1.08954
H	0.50350	-2.21174	0.55156
H	2.85736	-1.67255	1.18810
H	2.83335	-2.72817	-0.21984
H	1.22140	0.81185	-1.49021
H	3.52271	1.49145	-0.88446
H	3.27472	0.95938	0.77369
H	3.22265	-0.81137	-1.73373
C	-3.14447	0.65832	1.03310
H	-4.18478	0.43792	1.29877
H	-2.51535	0.40219	1.89376
H	-3.05556	1.72751	0.82414
C	-2.80184	-1.64676	-0.03177
H	-2.16728	-1.97968	0.79873
H	-3.82956	-1.96009	0.18451
H	-2.47473	-2.13140	-0.95521
H	4.46678	-0.81344	-0.48774

C	0.54848	0.17035	1.86479
H	0.08722	1.13579	2.09063
H	-0.05576	-0.61727	2.32820
H	1.53234	0.15513	2.35591
C	1.06329	2.44336	-0.11519
H	1.55818	3.13268	-0.80852
H	-0.01824	2.57687	-0.22065
H	1.35378	2.73606	0.90086

4-ax-TS:

C	-0.75824	0.68011	0.45079
C	-1.63846	0.70337	-0.80649
C	-1.92097	-0.72991	-1.31282
C	-2.45168	-1.66217	-0.21265
C	-1.48521	-1.71187	0.97891
C	-1.19664	-0.30549	1.52775
H	-1.07580	1.23280	-1.58779
H	0.32248	0.14514	-0.00536
H	-3.44171	-1.32608	0.12765
H	-2.10803	0.10136	1.99902
O	1.21355	-0.51072	-0.56069
C	2.56118	-0.16000	-0.22402
O	2.99327	-1.15452	-1.06251
H	-0.98793	-1.14551	-1.71067
H	-2.63113	-0.68144	-2.14832
H	-0.53824	-2.16323	0.65899
H	-0.44070	-0.34689	2.32220
H	-1.89064	-2.34277	1.77950
C	2.94478	1.23963	-0.70421
H	2.47379	2.02215	-0.09851
H	4.03095	1.37110	-0.63919
H	2.63980	1.35431	-1.74752
C	2.88591	-0.42345	1.24685

H	3.96632	-0.34326	1.41292
H	2.39054	0.29739	1.90885
H	2.56570	-1.43528	1.50815
H	-2.59343	-2.67000	-0.62186
C	-0.31074	2.03205	0.97394
H	-1.14367	2.53749	1.48310
H	0.49603	1.93167	1.70872
H	0.03253	2.68814	0.16683
C	-2.94342	1.50134	-0.57540
H	-2.74096	2.54386	-0.30887
H	-3.53888	1.50418	-1.49544
H	-3.56058	1.06515	0.21734

5-TS:

O	-3.28381	-0.01891	-1.44607
C	-2.66995	0.04073	-0.21991
O	-1.41182	-0.14661	-0.86998
C	2.97514	-1.18235	-0.27623
C	1.43685	-1.25157	-0.42565
C	0.76144	-0.12996	0.35457
C	1.28326	1.24813	-0.03464
C	2.82188	1.32023	0.11395
C	3.51167	0.19934	-0.67667
H	-0.42735	-0.13761	-0.13116
H	1.17894	-1.15069	-1.48777
H	1.06220	-2.22785	-0.09691
H	3.43227	-1.96694	-0.89161
H	1.01850	1.44377	-1.08155
H	0.80397	2.02765	0.56948
H	3.17031	2.30312	-0.22648
H	3.33970	0.35632	-1.75140
C	-2.78676	1.41107	0.44948
H	-3.82482	1.59689	0.74807

H	-2.16184	1.47772	1.34862
H	-2.48269	2.18325	-0.26183
C	-3.03856	-1.12833	0.69447
H	-2.42920	-1.13877	1.60608
H	-4.09043	-1.05447	0.99355
H	-2.89325	-2.06484	0.14999
H	4.59748	0.24246	-0.52359
C	0.58364	-0.37598	1.84188
H	-0.01408	0.41215	2.31318
H	0.10433	-1.34173	2.03481
H	1.55935	-0.38912	2.34938
H	3.25527	-1.39864	0.76418
H	3.09470	1.24363	1.17583

6-TS:

O	3.61876	-0.58868	-1.19386
C	2.93499	0.06433	-0.19973
O	1.75139	-0.61160	-0.62645
C	-2.60776	0.83029	-0.72746
C	-1.05360	0.81950	-0.63094
C	-0.49716	-0.18427	0.37535
C	-1.05326	-1.58889	0.17085
C	-2.59842	-1.57735	0.15828
C	-3.13373	-0.60955	-0.90707
H	0.71044	-0.31684	-0.01627
H	-0.66118	0.54891	-1.61966
H	-0.68502	1.82892	-0.40989
H	-2.84758	1.39024	-1.64229
H	-0.69672	-1.97470	-0.79310
H	-0.67667	-2.26715	0.94523
H	-2.96332	-2.59299	-0.03805
H	-2.82982	-0.97727	-1.89747
C	3.37547	-0.34651	1.20551

H	4.39363	0.01035	1.39867
H	2.71920	0.07422	1.97659
H	3.36644	-1.43716	1.27635
C	2.85602	1.57739	-0.40708
H	2.17236	2.04925	0.30932
H	3.84609	2.02790	-0.27296
H	2.51248	1.78112	-1.42446
H	-4.23163	-0.60704	-0.89931
C	-0.36805	0.26594	1.82051
H	0.25816	-0.42662	2.39390
H	0.06318	1.27014	1.89577
H	-1.35029	0.29458	2.31188
C	-3.29478	1.57006	0.43148
H	-2.88442	2.57945	0.55348
H	-4.36906	1.66965	0.23512
H	-3.18797	1.05274	1.39061
H	-2.97778	-1.30114	1.15096

7-TS:

O	3.85524	-0.22176	-1.30994
C	3.19807	0.00365	-0.12745
O	1.97688	-0.25377	-0.82068
C	-2.28343	1.36405	-0.53205
C	-0.74111	1.23092	-0.37962
C	-0.28406	-0.08732	0.23796
C	-0.87828	-1.30431	-0.46517
C	-2.42510	-1.26002	-0.62084
C	-2.86283	0.10102	-1.21025
H	0.92490	-0.14980	-0.14948
H	-0.30016	1.29478	-1.38275
H	-0.34557	2.07985	0.19173
H	-2.43870	2.19242	-1.23805
H	-0.44352	-1.34863	-1.47214

H	-0.57589	-2.22635	0.04617
H	-2.66641	-2.01606	-1.38162
H	-2.54249	0.11908	-2.26148
C	3.50153	-1.04246	0.94496
H	4.53857	-0.94132	1.28510
H	2.84832	-0.92939	1.81837
H	3.36787	-2.03962	0.51787
C	3.30431	1.44701	0.36511
H	2.63665	1.63543	1.21480
H	4.32927	1.65898	0.69043
H	3.04900	2.12383	-0.45419
H	-3.95948	0.16116	-1.22508
C	-0.16457	-0.14601	1.75141
H	0.31694	-1.07538	2.07463
H	0.41574	0.69968	2.13789
H	-1.14961	-0.10652	2.23335
C	-2.99873	1.78473	0.76225
H	-2.59645	2.73621	1.13085
H	-4.07020	1.92830	0.57763
H	-2.90484	1.05516	1.57081
C	-3.18584	-1.69141	0.64391
H	-4.26700	-1.68958	0.45979
H	-2.90097	-2.71065	0.93169
H	-3.00279	-1.04635	1.50727

8-TS:

O	-1.83101	2.78062	-0.43005
C	-0.49151	2.91192	-0.71440
O	-0.27488	2.02689	0.39001
C	3.50182	-0.99209	-0.07110
C	2.07014	-0.32363	-0.17630
C	1.85286	0.78585	0.86499
C	2.94424	1.85154	0.79383

C	4.35073	1.23114	0.92859
C	4.56676	0.13078	-0.11769
H	0.82408	1.39295	0.45474
H	2.07794	0.18505	-1.15320
H	2.89123	2.36224	-0.17812
H	2.78016	2.61268	1.56522
H	5.10409	2.01877	0.80461
H	4.55191	0.58888	-1.11766
C	-0.07848	2.33561	-2.06584
H	-0.52258	2.93635	-2.86739
H	1.01044	2.35926	-2.19579
H	-0.42807	1.30531	-2.15607
C	0.04923	4.31334	-0.44614
H	1.14497	4.32809	-0.47619
H	-0.32079	5.01342	-1.20371
H	-0.28866	4.64622	0.53821
H	5.56376	-0.31394	0.00335
C	1.41375	0.41169	2.27416
H	1.02492	1.29751	2.78652
H	0.63392	-0.35408	2.28182
H	2.25748	0.03594	2.86642
C	3.70541	-1.83890	1.20601
H	2.91512	-2.57828	1.36073
H	4.65310	-2.38598	1.12933
H	3.75852	-1.23087	2.11187
H	4.48720	0.83432	1.94185
C	0.96199	-1.39238	-0.26098
H	0.88722	-1.96950	0.66277
C	3.67031	-1.90519	-1.31282
H	3.66273	-1.27648	-2.21514
H	4.65935	-2.38119	-1.27340
C	1.17743	-2.33215	-1.45075
C	2.57298	-2.97074	-1.44036

H	2.72102	-3.54632	-2.36198
H	2.64761	-3.69207	-0.61680
H	0.39408	-3.09831	-1.44224
H	1.04419	-1.74744	-2.37150
O	-0.29613	-0.71021	-0.45332
C	-1.33417	-1.05148	0.36453
O	-1.30818	-1.97990	1.15699
N	-2.38421	-0.20921	0.15205
H	-2.18687	0.69069	-0.28221
C	-3.57400	-0.31503	0.95928
H	-3.81318	0.64773	1.42276
H	-3.41061	-1.05779	1.74293
C	-4.78251	-0.74538	0.14280
F	-4.60801	-1.95573	-0.42047
F	-5.05029	0.13074	-0.84912
F	-5.87671	-0.81137	0.93603

9-TS:

O	-1.51000	2.82885	-0.25192
C	-0.18850	2.89315	-0.63295
O	0.08848	2.05615	0.49458
C	3.54029	-1.27567	-0.02674
C	2.18380	-0.50385	-0.15167
C	2.17480	0.70289	0.80068
C	3.34818	1.64232	0.54565
C	4.69010	0.89096	0.69047
C	4.73209	-0.32714	-0.23798
H	1.15090	1.37598	0.47540
H	2.14089	-0.11227	-1.17985
H	3.28557	2.04273	-0.47604
H	3.30631	2.49610	1.23142
H	5.51651	1.57579	0.46443
H	4.73402	0.01422	-1.28418

C	0.10481	2.24005	-1.98152
H	-0.37750	2.81868	-2.77714
H	1.18132	2.21881	-2.19065
H	-0.28365	1.21999	-1.99609
C	0.41608	4.28564	-0.47522
H	1.50639	4.25786	-0.58601
H	0.01387	4.96290	-1.23713
H	0.16388	4.67594	0.51369
H	5.66813	-0.88184	-0.09183
C	1.89079	0.42413	2.26948
H	1.88823	1.35733	2.84077
H	0.92195	-0.06114	2.41397
H	2.65837	-0.23235	2.70251
H	3.60038	-1.67902	0.99651
H	4.82332	0.57231	1.73276
C	3.58052	-2.46504	-1.00232
H	4.52243	-3.01171	-0.86206
H	3.59346	-2.07994	-2.03298
C	0.99938	-1.47096	0.01621
H	0.96031	-1.86340	1.03698
C	2.38383	-3.40735	-0.82578
C	1.06031	-2.64415	-0.96257
H	2.42760	-4.21898	-1.56164
H	2.43409	-3.88264	0.16434
H	0.95487	-2.25382	-1.98428
H	0.20436	-3.29937	-0.77209
O	-0.19706	-0.70066	-0.21667
C	-1.30676	-1.03662	0.50259
O	-1.39609	-2.03661	1.19595
N	-2.27462	-0.09510	0.32078
H	-2.00508	0.81442	-0.05273
C	-3.54777	-0.21920	0.98225
H	-3.48849	-1.01621	1.72663

H	-3.81686	0.71725	1.48130
C	-4.66920	-0.56228	0.01289
F	-4.45539	-1.73574	-0.61170
F	-5.84400	-0.65420	0.67757
F	-4.81199	0.38493	-0.93898

10-eq-C2-TS:

O	5.43309	-1.69296	-1.18846
C	4.75295	-1.22453	-0.08431
O	3.70144	-0.73211	-0.91426
C	0.33925	2.47047	-0.22787
C	1.67063	1.70171	-0.53296
C	1.79026	0.40177	0.22314
C	0.64460	-0.56053	0.01358
C	-0.71534	0.10101	0.40523
C	-0.84237	1.45647	-0.39611
H	2.83232	-0.19434	-0.30050
H	1.69436	1.48306	-1.60918
H	2.52482	2.35564	-0.32217
H	0.60945	-0.84710	-1.04606
H	0.79559	-1.47991	0.59155
H	-0.75758	1.14308	-1.44948
H	2.12144	0.50434	1.26118
C	4.28427	-2.34857	0.84241
H	5.14571	-2.83444	1.31440
H	3.63382	-1.96904	1.64004
H	3.74042	-3.09196	0.25397
C	5.49995	-0.10083	0.63777
H	4.89086	0.34318	1.43456
H	6.41735	-0.48970	1.09393
H	5.76770	0.67219	-0.08698
C	0.41381	3.15495	1.15261
H	1.18760	3.93188	1.13953

H	-0.53332	3.64539	1.40379
H	0.65775	2.46719	1.96485
C	-0.77390	0.22096	1.94650
H	-1.47285	0.98427	2.29239
H	-1.07808	-0.73224	2.39305
H	0.20175	0.46546	2.37248
C	0.22798	3.58595	-1.29208
H	-0.58574	4.28416	-1.06962
H	1.15528	4.17006	-1.32428
H	0.05939	3.17341	-2.29416
C	-1.86456	-0.76929	-0.15828
C	-2.25736	2.07417	-0.27329
H	-2.30985	2.98865	-0.87175
H	-2.45465	2.38163	0.76105
C	-3.29579	-0.19836	0.00256
C	-3.37945	1.12307	-0.75733
H	-4.35983	1.59571	-0.62289
H	-3.26086	0.92319	-1.82957
O	-4.08309	-1.25404	-0.63989
C	-3.47391	-2.46655	-0.44306
O	-3.99302	-3.50514	-0.75458
C	-3.88737	-0.06560	1.41512
H	-4.97403	0.01484	1.31115
H	-3.67959	-0.93856	2.04101
H	-3.53336	0.82299	1.94071
C	-2.08381	-2.24623	0.17265
H	-2.12202	-2.46534	1.24662
H	-1.36975	-2.93648	-0.28209
H	-1.71049	-0.75746	-1.24770

10-ax-C3-TS:

C	1.15968	1.84897	-0.08842
C	2.04674	1.04209	0.86423

C	1.40366	0.37236	2.05861
C	0.14946	-0.42759	1.67566
C	-0.87389	0.40932	0.86722
C	-0.12768	1.00696	-0.39118
H	2.99907	1.53808	1.08737
H	0.46768	-1.28928	1.07553
H	-0.32340	-0.82483	2.58303
H	0.27253	0.11938	-0.90285
H	1.15911	1.15105	2.79921
C	0.89263	3.23791	0.55240
H	1.83118	3.79862	0.63277
H	0.21538	3.82371	-0.07927
H	0.45504	3.17895	1.55032
C	-1.52831	1.44275	1.81560
H	-1.93986	2.30972	1.29549
H	-2.34461	0.97909	2.38049
H	-0.81893	1.82170	2.55560
C	1.95199	2.09977	-1.39448
H	1.43956	2.81513	-2.04473
H	2.93628	2.52428	-1.16144
H	2.11111	1.17003	-1.94820
C	-1.91671	-0.55284	0.24596
C	-1.10408	1.65433	-1.40338
H	-0.54622	2.01571	-2.27264
H	-1.58632	2.53855	-0.96768
C	-2.94276	0.07969	-0.72551
C	-2.18593	0.67055	-1.91224
H	-2.86808	1.18330	-2.60115
H	-1.71258	-0.14534	-2.47209
O	-3.72724	-1.09911	-1.10294
C	-3.77317	-1.97515	-0.05002
O	-4.47033	-2.95507	-0.05816
C	-3.97093	1.07775	-0.16855

H	-4.78624	1.15390	-0.89509
H	-4.40438	0.74711	0.78015
H	-3.55541	2.07622	-0.02276
C	-2.80269	-1.50968	1.04570
H	-3.36942	-1.02941	1.85309
H	-2.28801	-2.37457	1.47015
H	-1.32669	-1.21403	-0.40598
H	2.12995	-0.28230	2.55480
H	2.46954	0.02712	0.14617
O	2.68080	-0.95491	-0.52118
C	4.01439	-1.46693	-0.40239
O	3.72284	-2.45683	-1.31170
C	4.30559	-2.01218	0.99675
H	4.39884	-1.20575	1.73425
H	3.49811	-2.68630	1.29387
H	5.24689	-2.57328	0.99277
C	5.06744	-0.48026	-0.90927
H	4.77921	-0.12496	-1.90171
H	5.17866	0.37666	-0.23426
H	6.04095	-0.97786	-0.98342

10-eq-C3-TS:

C	1.07586	1.08804	-0.03004
C	1.77116	-0.25076	-0.28912
C	1.27088	-1.46399	0.45740
C	-0.23373	-1.67223	0.15588
C	-1.08406	-0.41719	0.47277
C	-0.45668	0.80758	-0.30275
H	1.90828	-0.44137	-1.36093
H	-0.34632	-1.92819	-0.90700
H	-0.59953	-2.53465	0.72829
H	-0.47177	0.48437	-1.35643
H	1.42914	-1.34567	1.53480

C	1.38499	1.63828	1.37981
H	2.44697	1.89161	1.44682
H	0.80895	2.54938	1.57461
H	1.16793	0.92873	2.17978
C	-1.18225	-0.26082	2.00982
H	-1.37699	0.76458	2.32756
H	-1.98750	-0.88826	2.40705
H	-0.26519	-0.57908	2.51004
C	1.61708	2.10653	-1.05884
H	1.25502	3.11973	-0.85941
H	2.71010	2.13188	-1.00462
H	1.33031	1.83820	-2.08349
C	-2.47902	-0.57934	-0.18179
C	-1.35598	2.06691	-0.25531
H	-0.89557	2.86809	-0.84072
H	-1.42929	2.44884	0.77007
C	-3.42436	0.64481	-0.09179
C	-2.77456	1.81557	-0.82451
H	-3.38201	2.72425	-0.73645
H	-2.70941	1.57183	-1.89231
O	-4.59919	0.13512	-0.80532
C	-4.70774	-1.21636	-0.60625
O	-5.66138	-1.84738	-0.97823
C	-3.95140	1.07402	1.28695
H	-4.83107	1.70442	1.12282
H	-4.26431	0.22276	1.89877
H	-3.22311	1.65315	1.85743
C	-3.44413	-1.73270	0.09808
H	-3.65839	-1.89125	1.16198
H	-3.15592	-2.69600	-0.32888
H	-2.27204	-0.65831	-1.25999
H	1.82875	-2.35761	0.15618
H	3.03350	-0.07278	0.07525

O	4.11882	0.24691	0.43117
C	5.17975	-0.48193	-0.19436
C	5.13261	-1.97565	0.13484
H	5.01782	-2.09994	1.21467
H	4.30541	-2.47917	-0.37999
H	6.06556	-2.45806	-0.17776
C	5.28880	-0.18592	-1.69166
H	4.45504	-0.62343	-2.25379
H	5.29962	0.89652	-1.84307
H	6.21925	-0.60510	-2.09113
O	6.11968	0.19427	0.55179

10-eq-C2-TS':

O	4.27250	-0.91074	-1.84214
C	3.80749	-0.61193	-0.59599
O	2.48649	-0.54165	-1.10985
C	-0.90009	2.47336	-0.08191
C	0.43329	1.74258	-0.46214
C	0.57539	0.39742	0.20574
C	-0.55944	-0.56429	-0.05812
C	-1.92146	0.05574	0.39980
C	-2.07322	1.46089	-0.30109
H	1.60051	-0.11753	-0.34328
H	0.43977	1.59562	-1.55033
H	1.28744	2.38264	-0.21949
H	-0.60897	-0.77508	-1.13465
H	-0.39341	-1.51972	0.45362
H	-2.00306	1.22248	-1.37494
H	0.90805	0.44268	1.24617
C	4.08117	-1.74970	0.44404
C	4.22930	0.83104	-0.18832
C	-0.80815	3.06673	1.33923
H	-0.04139	3.85006	1.36303

H	-1.75523	3.53093	1.63653
H	-0.54352	2.33246	2.10286
C	-1.95703	0.06488	1.94648
H	-2.66302	0.78951	2.35571
H	-2.23867	-0.92271	2.32821
H	-0.97938	0.29561	2.37507
C	-1.03877	3.65601	-1.06777
H	-1.85370	4.33061	-0.78469
H	-0.11672	4.24876	-1.07760
H	-1.22283	3.30913	-2.09168
C	-3.06886	-0.78729	-0.20752
C	-3.49252	2.05348	-0.11406
H	-3.56233	3.00699	-0.64592
H	-3.67689	2.28630	0.94200
C	-4.50371	-0.24471	0.01243
C	-4.61144	1.12660	-0.64884
H	-5.59470	1.57655	-0.46691
H	-4.50687	1.00526	-1.73414
O	-5.28796	-1.26051	-0.69490
C	-4.66488	-2.47732	-0.59091
O	-5.17746	-3.49714	-0.96802
C	-5.07852	-0.22165	1.43794
H	-6.16704	-0.14414	1.35280
H	-4.85586	-1.13580	1.99638
H	-4.72602	0.62932	2.02315
C	-3.26853	-2.28613	0.02116
H	-3.28934	-2.58225	1.07719
H	-2.55452	-2.93477	-0.49137
H	-2.93069	-0.69707	-1.29540
C	3.64279	-1.39472	1.87795
H	3.81007	-2.26195	2.52712
H	4.20694	-0.55573	2.29446
H	2.57633	-1.14861	1.93066

C	5.59266	-2.07536	0.43495
H	5.93527	-2.30467	-0.57960
H	6.19623	-1.25221	0.82410
H	5.77966	-2.95574	1.06040
C	3.30994	-2.99991	-0.02663
H	3.55424	-3.24062	-1.06443
H	3.58148	-3.85410	0.60380
H	2.22724	-2.85722	0.04017
F	3.47377	1.29977	0.84707
F	4.06053	1.68586	-1.20524
F	5.51906	0.90449	0.20059

10-ax-C3-TS':

C	0.14457	-2.07096	0.36159
C	-0.79119	-1.22166	1.22858
C	-0.16701	-0.31481	2.26661
C	0.96874	0.54615	1.69534
C	2.04125	-0.29013	0.95360
C	1.31077	-1.15598	-0.14776
H	-1.66491	-1.77628	1.58680
H	0.53129	1.27313	0.99876
H	1.43593	1.12152	2.50468
H	0.78639	-0.40911	-0.76219
H	0.20334	-0.95235	3.08574
C	0.59709	-3.28999	1.21367
H	-0.26533	-3.92776	1.43855
H	1.31440	-3.89623	0.64921
H	1.06223	-3.01131	2.16057
C	2.86365	-1.08226	1.99905
H	3.32438	-1.98605	1.59577
H	3.66598	-0.45770	2.40666
H	2.25215	-1.39074	2.85107
C	-0.65573	-2.63698	-0.83564

H	-0.08880	-3.41226	-1.35985
H	-1.58829	-3.09375	-0.48664
H	-0.92154	-1.85383	-1.54976
C	2.92895	0.67105	0.12346
C	2.30606	-1.84536	-1.11298
H	1.75154	-2.39809	-1.87711
H	2.91065	-2.59198	-0.58239
C	3.97458	0.00998	-0.80647
C	3.23785	-0.84186	-1.83690
H	3.94226	-1.37963	-2.48277
H	2.64419	-0.18315	-2.48236
O	4.59281	1.19331	-1.41121
C	4.58318	2.22620	-0.51130
O	5.15447	3.26436	-0.71656
C	5.14116	-0.76827	-0.17693
H	5.91922	-0.87241	-0.93991
H	5.58419	-0.24590	0.67648
H	4.85376	-1.76916	0.14921
C	3.73029	1.83686	0.70554
H	4.38905	1.55997	1.53807
H	3.13646	2.69649	1.02419
H	2.23187	1.14909	-0.58062
H	-0.93423	0.32137	2.72281
H	-1.37111	-0.41718	0.41207
O	-1.70654	0.42082	-0.45460
C	-3.08746	0.75611	-0.58930
O	-2.78882	1.47341	-1.70460
C	-3.70532	1.63082	0.55241
C	-3.85655	-0.54908	-0.95464
C	-4.15632	0.81230	1.77758
H	-4.97223	0.12367	1.54115
H	-3.33541	0.22919	2.20995
H	-4.51523	1.49762	2.55397

C	-2.64200	2.66110	0.98335
H	-3.09547	3.38952	1.66496
H	-1.80289	2.19027	1.50328
H	-2.24618	3.19677	0.11658
C	-4.91521	2.40380	-0.02429
H	-4.62115	2.98179	-0.90665
H	-5.73656	1.74129	-0.30475
H	-5.29034	3.10648	0.72851
F	-3.74775	-1.48017	0.03430
F	-5.17522	-0.33762	-1.15124
F	-3.36736	-1.10341	-2.07148

10-eq-C3-TS':

C	0.16665	-1.13894	0.39718
C	-0.59010	0.12305	-0.02721
C	-0.08836	1.45008	0.49087
C	1.38344	1.65320	0.05325
C	2.30093	0.48727	0.49255
C	1.66668	-0.85834	-0.03438
H	-0.79522	0.13797	-1.10360
H	1.41425	1.74877	-1.04106
H	1.74942	2.60372	0.46294
H	1.59096	-0.70640	-1.12315
H	-0.16823	1.49272	1.58226
C	-0.01753	-1.45418	1.89752
H	-1.05314	-1.75403	2.08159
H	0.63054	-2.28339	2.20042
H	0.19749	-0.60633	2.55010
C	2.52110	0.57432	2.02206
H	2.76480	-0.38650	2.47813
H	3.33861	1.26601	2.25187
H	1.63836	0.95630	2.53950
C	-0.38913	-2.33489	-0.40763

H	0.04762	-3.28102	-0.07454
H	-1.47048	-2.41114	-0.26899
H	-0.19221	-2.22734	-1.48147
C	3.63512	0.58427	-0.29112
C	2.61576	-2.06966	0.13683
H	2.14632	-2.96622	-0.27698
H	2.78179	-2.28119	1.19999
C	4.63330	-0.58361	-0.09371
C	3.97465	-1.87268	-0.57917
H	4.62184	-2.73963	-0.40056
H	3.81794	-1.80387	-1.66290
O	5.72603	-0.15922	-0.97323
C	5.79577	1.20954	-0.99156
O	6.69093	1.80141	-1.53372
C	5.28391	-0.77660	1.28547
H	6.16782	-1.40749	1.14845
H	5.61709	0.16743	1.72684
H	4.62342	-1.27123	1.99974
C	4.57141	1.79367	-0.27044
H	4.86116	2.11977	0.73588
H	4.21214	2.67115	-0.81288
H	3.34305	0.48899	-1.34786
H	-0.69763	2.27119	0.09823
H	-1.79448	-0.01467	0.41573
O	-2.85069	-0.23507	1.01511
C	-4.08405	-0.01571	0.33718
C	-4.46367	1.47744	0.05472
C	-4.13123	-0.98389	-0.88209
O	-4.76303	-0.54084	1.39324
F	-3.96158	-2.25710	-0.49318
F	-5.30068	-0.91832	-1.55207
F	-3.14271	-0.70973	-1.77801
C	-3.81159	2.04842	-1.21940

H	-4.16086	1.54809	-2.12694
H	-4.06703	3.11071	-1.30722
H	-2.71882	1.97503	-1.19285
C	-4.02234	2.30798	1.27697
H	-4.39211	3.33430	1.17321
H	-4.42642	1.88411	2.20010
H	-2.93366	2.34657	1.37289
C	-6.00215	1.57926	-0.06811
H	-6.29204	2.63328	-0.14814
H	-6.38430	1.05758	-0.94830
H	-6.49056	1.16275	0.81902

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